

2-Chlorobenzoic acid, 2-butyl ester

Other names:	Benzoic acid, 2-chloro, 1-methylpropyl ester
Inchi:	InChI=1S/C11H13ClO2/c1-3-8(2)14-11(13)9-6-4-5-7-10(9)12/h4-8H,3H2,1-2H3
InchiKey:	PSVMSRFFQPHGTG-UHFFFAOYSA-N
Formula:	C11H13ClO2
SMILES:	CCC(C)OC(=O)c1ccccc1Cl
Mol. weight [g/mol]:	212.67
CAS:	97989-28-1

Physical Properties

Property code	Value	Unit	Source
gf	-103.77	kJ/mol	Joback Method
hf	-311.13	kJ/mol	Joback Method
hfus	21.36	kJ/mol	Joback Method
hvap	56.17	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.295		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	1446.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1450.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2067.00		NIST Webbook
ripol	2054.00		NIST Webbook
ripol	2031.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2030.00		NIST Webbook
tb	596.02	K	Joback Method
tc	814.94	K	Joback Method
tf	339.75	K	Joback Method
vc	0.611	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.26	J/molxK	596.02	Joback Method
cpg	433.43	J/molxK	778.45	Joback Method
cpg	422.97	J/molxK	741.97	Joback Method
cpg	411.74	J/molxK	705.48	Joback Method
cpg	399.73	J/molxK	668.99	Joback Method
cpg	386.90	J/molxK	632.51	Joback Method
cpg	443.15	J/molxK	814.94	Joback Method
dvisc	0.0001789	Paxs	596.02	Joback Method
dvisc	0.0002290	Paxs	553.31	Joback Method
dvisc	0.0003054	Paxs	510.60	Joback Method
dvisc	0.0004294	Paxs	467.88	Joback Method
dvisc	0.0006465	Paxs	425.17	Joback Method
dvisc	0.0010666	Paxs	382.46	Joback Method
dvisc	0.0019955	Paxs	339.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97989281&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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